

1-Pentanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,5-undecafluoro-
2706-91-4 | DTXSID8062600

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 1050 L/kg

Global applicability domain: Outside

Local applicability domain index: 3.50e-01

Confidence level: 5.20e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Tetrachlorophthalic acid</div> <div>Measured: 2000</div> <div>Predicted: 1980</div>	<div>Image not found</div> <div>Chlorothalonil</div> <div>Measured: 1820</div> <div>Predicted: 1300</div>	<div>Image not found</div> <div>Fthalide</div> <div>Measured: 2000</div> <div>Predicted: 1600</div>
<div>Image not found</div> <div>Sulfone, methyl pentafluorophenyl</div> <div>Measured: 28.8</div> <div>Predicted: 104</div>	<div>Image not found</div> <div>Chlorthal-dimethyl</div> <div>Measured: 5010</div> <div>Predicted: 2160</div>	